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L6 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2006:693745 CAPLUS

DN 145:336301

TI Modification of guanine residues in PNA-synthesis by PyBOP

AU Pritz, Stephan; Wolf, Yvonne; Klemm, Clementine; Bienert, Michael

CS Leibniz-Institute of Molecular Pharmacology, Berlin, 13125, Germany

SO Tetrahedron Letters (2006), 47(33), 5893-5896 CODEN: TELEAY; ISSN: 0040-4039

PB Elsevier B.V.

DT Journal

LA English

OS CASREACT 145:336301

AB The phosphonium-type coupling reagent PyBOP, when applied to the synthesis

of peptide nucleic acid (PNA) oligomers, was found to form O4-phosphonium compds. of the nucleobase guanine which can be converted into C4-modified guanine-derived PNAs by nucleophiles.

IT 105047-45-8

RL: RCT (Reactant); RACT (Reactant or reagent)
(PNA-synthesis using PyBOP as coupling reagent and determination of guanine-modified byproducts by MS/MS-fragmentation)

RN 105047-45-8 CAPLUS

CN L-Lysine, N2-[(9H-fluoren-9-ylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2006:152794 CAPLUS

DN 144:391376

TI An efficient, convenient solid-phase synthesis of amino acid-modified peptide nucleic acid monomers and oligomers

AU Balaji, Baghavathy S.; Gallazzi, Fabio; Jia, Fang; Lewis, Michael R.

CS Department of Veterinary Medicine and Surgery, Molecular Biology Program, Department of Radiology, and Nuclear Science and Engineering Institute, University of Missouri-Columbia, Columbia, MO, 65211, USA

SO Bioconjugate Chemistry (2006), 17(2), 551-558 CODEN: BCCHES; ISSN: 1043-1802

PB American Chemical Society

DT Journal

LA English

An efficient and highly versatile method for the synthesis of amino AΒ acid-modified peptide nucleic acid (PNA) monomers is described. By using solid-phase Fmoc (Fmoc = 9-fluorenylmethyloxycarbonyl) techniques, such monomers can be assembled readily in a stepwise manner and obtained in high yield with minimal purification Protected neutral hydrophilic, acidic, and basic amino acids were coupled to 2-chlorotrityl chloride resin. Following Fmoc removal, innovative conditions for the key step, reductive alkylation with N-Fmoc -aminoacetaldehyde, were developed to circumvent problems encountered with previously reported methods. Activation and coupling of pyrimidine and purine nucleobases to the resulting secondary amines afforded amino acid-modified PNA monomers. The mild reaction conditions utilized were compatible with sensitive and labile functional groups, such as tert-Bu ethers and tert-Bu esters. PNA monomers were obtained in 36-42% overall yield and very high purity, after cleavage and purification Using standard solid-phase Fmoc chemical, two of these monomers were incorporated with high coupling efficiency into a variety of modified PNA oligomers, including four tetradecamers designed to target bcl-2 mRNA. Such modified oligomers have the potential to enhance water solubility and cell portability, while maintaining hybridization affinity and promoting favorable biodistribution properties. ΙT 71989-26-9

RL: RCT (Reactant); RACT (Reactant or reagent)
 (solid phase synthesis of peptide nucleic acid monomers and oligomers
 via reductive alkylation with aminoacetaldehyde as key step)
71989-26-9 CAPLUS
L-Lysine, N6-[(1,1-dimethylethoxy)carbonyl]-N2-[(9H-fluoren-9ylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN

CN

IT 882780-21-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (solid phase synthesis of peptide nucleic acid monomers and oligomers via reductive alkylation with aminoacetaldehyde as key step)

RN 882780-21-4 CAPLUS

CN 13-Oxa-2,5,11-triazapentadecanoic acid, 6-carboxy-5-[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-14,14-dimethyl-12-oxo-, 1-(9H-fluoren-9-ylmethyl) ester, (6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2004:905902 CAPLUS

DN 141:380101

TI Novel functional peptide nucleic acid and process for producing the same

IN Tonosaki, Madoka; Ikeda, Hisafumi

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PA Credia Japan Co., Ltd., Japan SO PCT Int. Appl., 36 pp. CODEN: PIXXD2
DT Patent
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LA Japanese FAN.CNT 1

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AB In a process for producing a functional PNA oligomer, a PNA monomer unit having protected adenine, guanine, cytosine or thymine is reacted with Boc-Lys(Fmoc)-OH or Fmoc-Lys(Alloc)-OH (Alloc = allyloxycarbonyl) to synthesize a PNA oligomer Then a functional mol. having a free carboxylic acid is transferred into the above PNA oligomer and the protecting group is deblocked. According to this method having a good cost performance, a functional mol. can be transferred at an extremely high speed. Moreover, this method makes it possible to synthesize the above compound and the Boc-Lys(Fmoc)-OH or Fmoc-Lys(Alloc)-OH serving as a precursor PNA monomer unit. Using this process, a membrane-permeable fluorescent PNA probe R-NH(CH2)6CO-Lys(R1)-Lys(R1)-Lys(R1)-NH(CH2)6CO-GCATCCCACTTCTCATCC (I; R = Q; R1 = H-L-Arg-L-Arg-L-Arg) was prepared ΙT 84624-27-1 104669-73-0

RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of novel functional peptide nucleic acid using N α -Boc- or N α - Fmoc-Lys(Fmoc or allyloxycarbonyl)-OH and PNA monomers)

RN 84624-27-1 CAPLUS

CN L-Lysine, N2-[(1,1-dimethylethoxy)carbonyl]-N6-[(9H-fluoren-9-ylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 104669-73-0 CAPLUS

Absolute stereochemistry.

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L6 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
- AN 2003:679388 CAPLUS
- DN 139:381726
- Modulation of the Pharmacokinetic Properties of PNA: Preparation of Galactosyl, Mannosyl, Fucosyl, N-Acetylgalactosaminyl, and N-Acetylglucosaminyl Derivatives of Aminoethylglycine Peptide Nucleic Acid Monomers and Their Incorporation into PNA Oligomers
- AU Hamzavi, Ramin; Dolle, Frederic; Tavitian, Bertrand; Dahl, Otto; Nielsen, Peter E.
- CS Center for Biomolecular Recognition, Department of Medical Biochemistry and Genetics, University of Copenhagen, Copenhagen, DK-2200, Den.
- SO Bioconjugate Chemistry (2003), 14(5), 941-954 CODEN: BCCHES; ISSN: 1043-1802
- PB American Chemical Society
- DT Journal
- LA English

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AR A series of N-(2-aminoethyl)- α -amino acid thymine peptide nucleic acid (PNA) monomers bearing glycosylated side chains in the lpha-amino acid position (e.g, I) have been synthesized. These include PNA monomers where glycine has been replaced by serine and threonine (O-glycosylated), derivs. of lysine and nor-alanine (C-glycosylated), and amide derivs. of aspartic acid (N-glycosylated). The Boc and Fmoc derivs. of these monomers were used for incorporation in PNA oligomers. Twelve PNA decamers containing the glycosylated units in one, two, or three positions were prepared, and the thermal stability (Tm) of their complexes with a complementary RNA was determined Incorporation of the glycosyl monomers reduced the duplex stability by $0-6^{\circ}$ C per substitution. A cysteine was attached to the amino terminus of eight of the PNA decamers (Cys-CTCATACTCT-NH2) for easy conjugation to a [18F]radiolabeled N-(4-fluorobenzyl)-2-bromoacetamide. The in vivo biodistribution of these PNA oligomers was determined in rat 2 h after i.v. administration. Most of the radioactivity was recovered in the kidneys and in the urine. However, N-acetylgalactosamine (and to a lesser extent galactose and mannose)-modified PNAs were effectively targeting the liver (40-fold over unmodified PNA). Thus, the pharmacodistribution in rats of PNA oligomers can be profoundly changed by glycosylation. These results could be of great significance for PNA drug development, as they should allow modulation and fine-tuning of the pharmacokinetic profile of a drug lead. TΨ 150629-67-7

Т

RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of glycosylated monomers for PNA synthesis and their effect on PNA/RNA hybridization or PNA biodistribution) 150629-67-7 CAPLUS

CN L-Lysine, N6-[1-(4,4-dimethyl-2,6-dioxocyclohexylidene)ethyl]-N2-[(9H-fluoren-9-ylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN

IT 612491-20-0P 612491-21-1P 612491-22-2P 612491-23-3P 612491-24-4P 612491-25-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of glycosylated monomers for PNA synthesis and their effect on PNA/RNA hybridization or PNA biodistribution)

RN 612491-20-0 CAPLUS

CN L-Lysine, N2-[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-N2[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-N6,N6-bis(1,3,4,5-tetra-0-acetyl-2,6-anhydro-7,8-dideoxy-D-glycero-L-galacto-octitol-8-yl)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

RN 612491-21-1 CAPLUS

CN L-Lysine, N2-[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-N2[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-N6,N6-bis(3,4,5-tri-0acetyl-2,6-anhydro-1,7,8-trideoxy-L-glycero-D-galacto-octitol-8-yl)- (9CI)
(CA INDEX NAME)

RN 612491-22-2 CAPLUS

CN L-Lysine, N2-[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-N2[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-N6-(4,5,6,8-tetra-O-acetyl3,7-anhydro-2-deoxy-D-glycero-L-gluco-octonoyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612491-23-3 CAPLUS

CN L-Lysine, N2-[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-N2[2-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]ethyl]-N6-(4,5,6,8-tetra-Oacetyl-3,7-anhydro-2-deoxy-D-glycero-L-gluco-octonoyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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RN 612491-25-5 CAPLUS CN L-Lysine, N2-[(3,4-dihydro-5-methyl-2,4-dioxo-1(20)) Paramid N2-[(3,4-dihydro-5-methyl-2,4-dioxo-1(20)) N2-[(3, [2-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]ethyl]-N6-(4,5,6,8-tetra-0acetyl=3.7=anhydro=2-deoxy=D=glycero-D-talo-octonoyl)- (9CI) NAME) "Totally" said lamicia as she crunched on her bacon. "Thank their delicious breakfast. "Ummh, delicious" said Rosemary

as she cut up her pancake streaming with maple syrup. The crunch of bacon filled the room as they due into

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DTJournal

LA English

ΙT

OS CASREACT 136:295013

AB The site-selective conjugation of peptide nucleic acids (PNA) with fluorescent reporter groups is essential for the construction of hybridization probes that can report the presence of a particular DNA sequence. -This paper-describes convergent-methods for the solution and solid-phase synthesis of multiply labeled PNA oligomers

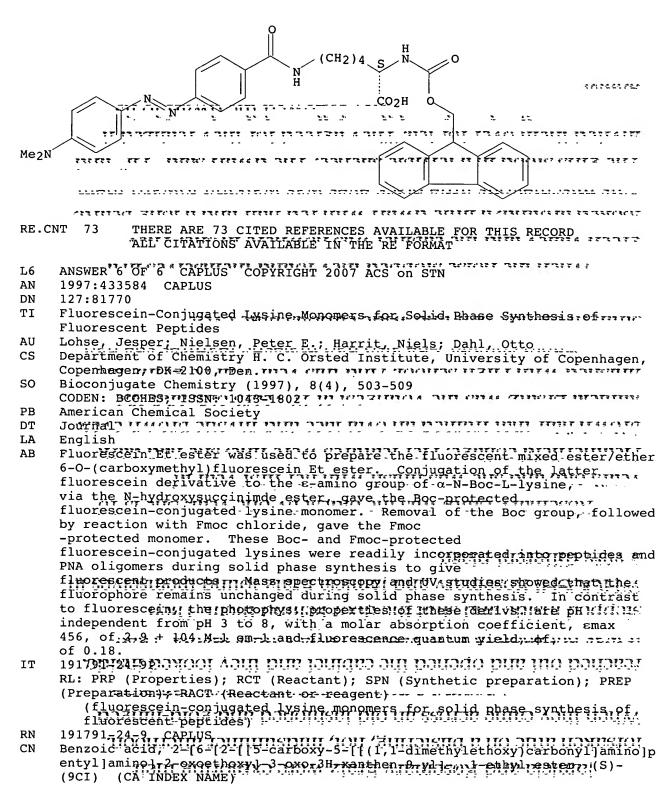
The replaid phase synthesis of grotestad PNA enabled the set of fluorescent labels at the C-terminal end (3' in DNA) which Ecarphane and the companion of the compa For the conjugation to internal sites, a method is introduced MIJO KHOHILICHISHUMMIKHIILDOHIDINGHISHILIHHER-UQAQUUTI BURIYAQRU omitting the need to synthesize an entire monomer in solution Furthermore, it is shown that the application of a highly orthogonal protecting group strategy in combination with chemoselective conjugation reactions provides accession and applied and all lands of the conjugation reactions provides accession and applied and all lands of the conjugation reactions provides accession. PNA probes. Real-time measurements of nucleic acid hybridization were possible by reached and and of the floorescence resonance energy transfer (FRET) between suitably appended fluorophoric groups. Analogously to DNA based moli beacons, the dual labeled TNA probes were only weakly fluorescing in the single-stranded state. Hybridization to a complementary oligonucleotide, however, induced a structural reorganization and conferred a virgith through the property of the second of the secon 146998-27-8

RL: RCT:(Reactant); RACT.(Reactant; or reagent) (convergent strategies for attachment of fluorescing reporter groups to DCGLOOMY MUICEEMOBING CHANGING AND SON I FOR SON POPEN THE COLORD PRINCES.

146998-27-8 CAPLUS RN CN L-Sychten.NG-141n[44-Chare Bydadlid bold] 14-2151 Behldyig CN2-C (Balve 1634 CA)

ylmethoxy)carbonyl]- (9CI) (CA INDEX NAME) | 1900 | 191.6C

Double bond geometry unknown.



IT 54613-99-9

RL: RCT (Reactant); RACT (Reactant or reagent)
(fluorescein-conjugated lysine monomers for solid phase synthesis of
fluorescent peptides)

RN 54613-99-9 CAPLUS

CN L-Lysine, N6-[[(2-chlorophenyl)methoxy]carbonyl]-N2-[(1,1dimethylethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 191791-27-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(fluorescein-conjugated lysine monomers for solid phase synthesis of fluorescent peptides)

RN 191791-27-2 CAPLUS

CN Benzoic acid, 2-[6-[2-[[5-carboxy-5-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]pentyl]amino]-2-oxoethoxy]-3-oxo-3H-xanthen-9-yl]-, 1-ethyl ester, (S)- (9CI) (CA INDEX NAME)